ANL-ART-197

Preliminary design analysis workflow for Division 5 HHA-3200 requirements for graphite core components

Applied Materials Division

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Argonne National Laboratory

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ABSTRACT

This report presents a design analysis workflow for graphite core components and assemblies, based on the design rules of ASME Boiler Pressure and Vessel Code, Section III, Division 5, Article HHA-3000. The workflow contains three stages: developing the design of the graphite core component, modeling the component with the finite element software MOOSE, and assessing if the component passes/fails the criteria of the HHA-3000 design rules. Since the design rules use probabilistic metrics specifically established to evaluate brittle materials, we developed a python library that performs all the statistical calculations necessary for the evaluations of the HHA-3000 criteria.

ACRONYMS AND ABBREVIATIONS

Acronym	Definition
ASME	American Society of Mechanical Engineers
BPVC	Boiler Pressure and Vessel Code
CDF	Cumulative Density Function
F	Non-dimensional parameter denoting the relative displacements per atom (dpa)
FEA	Finite Element Analysis
HHA	Subsection HH, Subpart A
MOOSE	Multiphysics Object-Oriented Simulation Environment
PDF	Probability Density Function
POF	Probability of Failure
POS	Probability of Survival
SRC	Structural Reliability Class
T	Non-dimensional parameter denoting the relative temperature
TRISO	TRIstructural ISOtropic
USNC	Ultra-Safe Nuclear Corporation

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1 Introduction

Graphite core components and assemblies have highly variable material properties with a nonlinear relationship to temperature and radiation (that is, sometimes graphite can actually have improved material properties at a higher temperature/radiation dose). As a result, the design analysis developed for graphite in ASME Section III, Division 5, Subsection HH, Subpart A (HHA) is probabilistic in nature, only considers the combined stresses present in the component, and demands the careful tracking of stresses over time. This is very different from the usual design rules for metallic components, which require the designer to differentiate between primary and secondary stresses (when elastic analysis approach is used), perform several deterministic assessments, and concentrate the analysis on the limiting temperatures (usually the highest) and loading conditions.

The design rules for graphite have separate design stress limits based on the safety importance and the absorbed neutron damage, instead of the usual limits for metallic components that are based on stress classifications. Structural Reliability Classes (SRCs) are also used by the designer to define the component's desired reliability. In other words, the SRC assigns an upper limit to the probability of failure (POF) that is acceptable on the graphite component. Additionally, the material strength (and therefore brittleness) is modeled with a Weibull distribution that describes the probability that, within each portion of the graphite billet, the strength will meet or exceed some minimum value. The Weibull distribution and the stress analysis, possibly obtained from a Finite Element Analysis (FEA), are used jointly to predict the POF of the entire component. Some amount of failure is expected to occur over time.

Given the complexity of the design evaluation for graphite core components and assemblies, we want to establish an easy-to-use design analysis workflow that complies with the requirements in HHA-3000 through the consideration of a sample problem for a prototypical 3D graphite core component. The following section demonstrates a full workflow that begins with the procedures needed to fully describe a graphite core, is followed by the calculation of stresses given a multi-physics model, and is ended with the calculation and visualization of POFs/stress limits that are derived from the Weibull distributions. This workflow not only allows the designer to evaluate whether the graphite core component passes the design criteria in HHA-3000, but also it enables the designer to locate critical locations where the component is most prone to failure.

2 Methodology

2.1 Design analysis workflow overview

The design analysis workflow for compliance with Division 5, paragraph HHA-3200 for graphite core components can be divided into three stages: the development of the design (the model), the modeling of the design, and the analysis of the design using the HHA-3200 rules. Figure 1 shows a full overview of the analysis workflow. Throughout these stages, we tried to use as much open-source software as possible and we tried to automate most of the process. Because of this automation, most of the designer's heavy work is done in the design development stage. All the tools that the designer needs to use throughout the workflow will be available in the online git repositories in the near future.

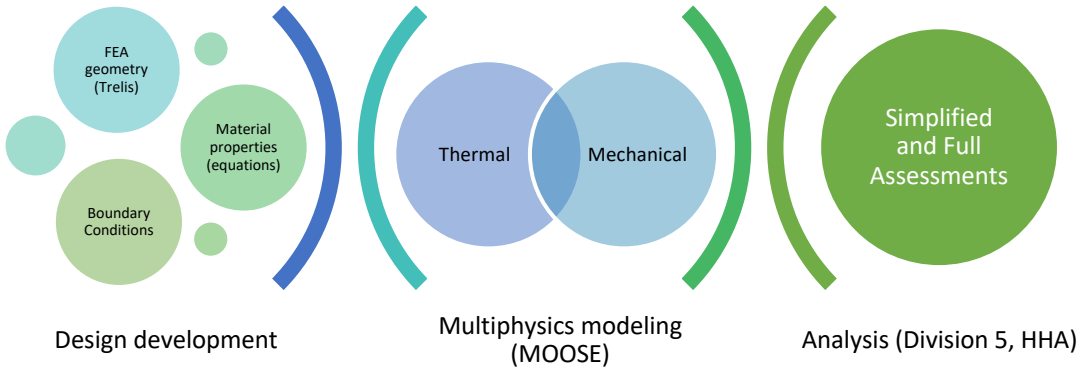

Figure 1: Overview of the design analysis workflow for graphite core components

2.2 Design development

To set up the problem that describes the design of a graphite core component, we require three groups of information: the geometry, the material properties, and the boundary conditions. The following section describes the different methodologies and procedures needed to obtain all three groups of information for a prismatic fuel block subject to conduction, convection, radiation, creep, swelling, thermal expansion, and other physical phenomena.

2.2.1.1 Geometry

In this work, the geometry used to model a graphite core component is based on reports that analyze prismatic blocks [1], [2]. The full geometry that we are using as baseline is shown in Figure 2, after [2].

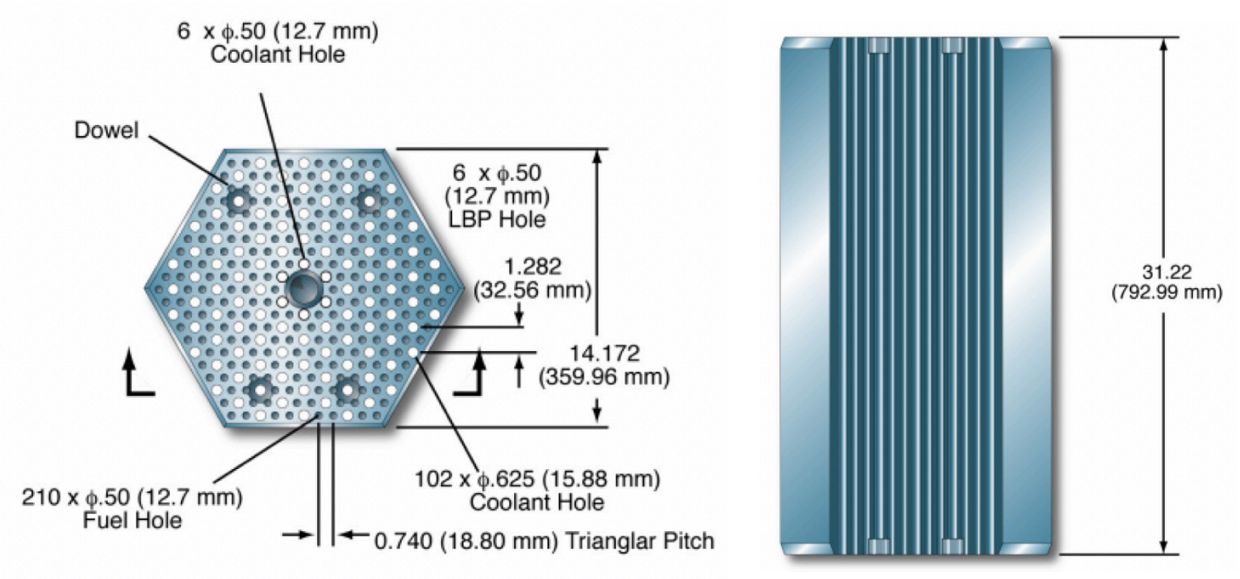

Figure 2: Original prismatic fuel block geometry (from [2]**).**

We generated both the geometry and the finite element mesh using Trelis, a meshing pre-processor based on Sandia National Laboratory's CUBIT mesher. The mesh can be generated using any other type of software, be it commercial or open-source, as long as the FEA mesh file is in the Exodus format (*.exo). To reduce the size of the problem, the actual FEA geometry is a 1/8th section of the full graphite core component and excludes chamfers as well as dowels. Figure 3 shows the final mesh (in mm), which contains 9861 HEX8 elements as well as 19256 nodes.

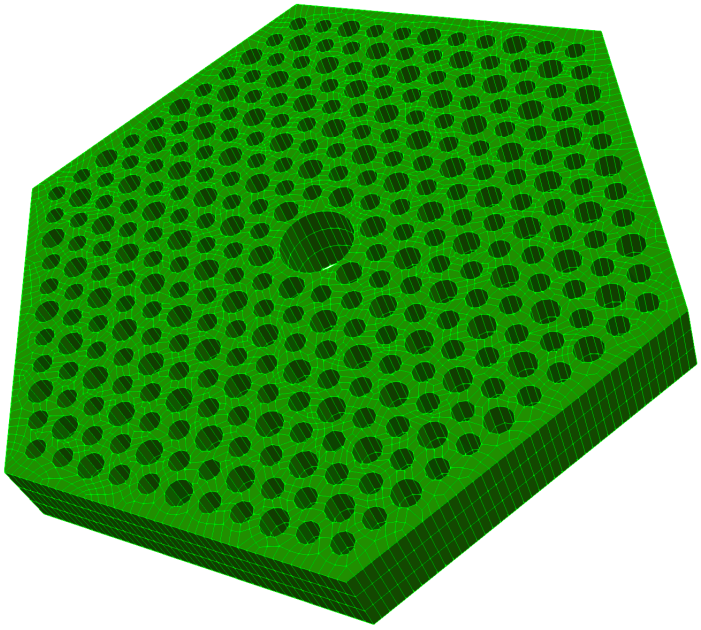

Figure 3: FEA model of 1/8th of a prismatic fuel element.

2.2.1.2 Material properties

The material used to model the graphite core component is ATR-2E, a material developed as a reference material for high temperature reactors. We obtained the material data from USNC's GitHub repository [3], which is based on a scientific report that characterized the data over a wide range of irradiation experiments [4]. Using the Jupyter notebook in the USNC's open-source package, we fitted a surface response onto the experimental data to find the relationships between the material properties of interest, temperature, and displacements per atom (dpa). We would like to note that graphite core components are three-dimensional solids that have one dimension larger than the other two, where the long axes will tend to take on a preferred orientation during forming in the direction of the extrusion. For a graphite core component manufactured via extrusion, as seen in Figure 4, X and Y are equivalent directions and are termed "against grain" or "perpendicular" directions. Properties will be symmetric about the Z axis and are termed "with-grain" or "parallel" direction.

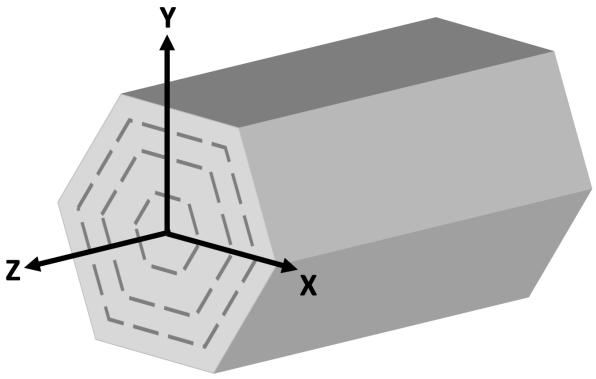

Figure 4. Orientations of graphite core component manufactured via extrusion

In the case of ATR-2E, we have a total of 5 material parameters that describe the response of the material given a certain temperature and/or dpa. Each of the material parameters has a different behavior in the "parallel" and the "perpendicular" direction, bringing the material parameter count to 10:

Parameter	Perpendicular	Parallel
Coefficient of thermal expansion (CTE_0) no dpa	$CTE_{o_{per}}$	$CTE_{o_{par}}$
Dimensional change (DL)	DL_{per}	DL_{par}
Conductivity (α)	α_{per}	α_{par}
Relative Young's Modulus E/E_o	$\left(\frac{E}{E_o}\right)_{per}$	$\left(\frac{E}{E_o}\right)_{par}$
Relative coefficient of Thermal expansion CTE/CTE_o	$\left(\frac{CTE}{CTE_o}\right)_{per}$	$\left(\frac{CTE}{CTE_o}\right)_{par}$

The baseline conductivity and Young's modulus, CTE_o and E_o respectively, are the baseline material properties of ATR-2E obtained in the absence of radiation. These parameters are used to populate the vectors and matrices representing the anisotropy of ATR-2E graphite as described in Section 2.3.3. To describe the parameters as a function of temperature and dpa, we fit an analytic surface response to the experimental data, as shown in Figure 5 for the material

parameters in the perpendicular direction. A similar fit was performed to the material parameters in the parallel direction.

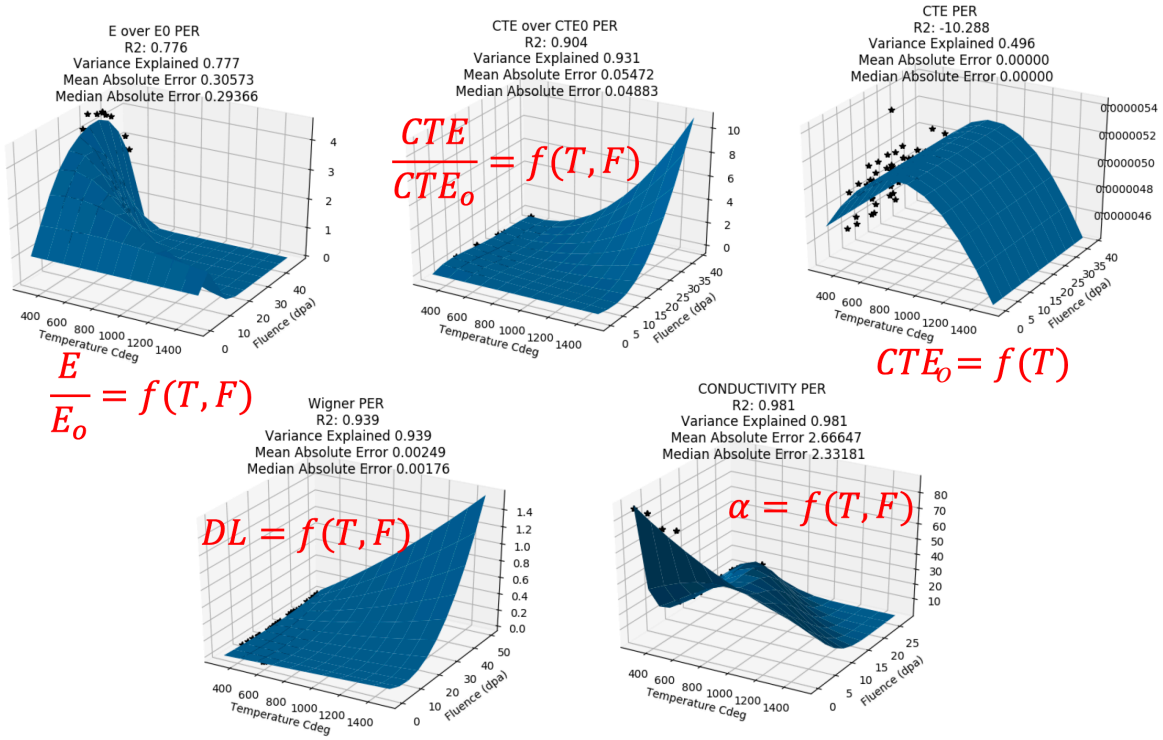

Figure 5: View of the 5 ATR-2E graphite material properties on the perpendicular build direction as a function of temperature (T) and dpa (F). A similar set of responses is obtained for the parallel build direction.

Polynomial equations can describe the surface responses, where the temperature and the dpa are transformed into unitless variables and the resulting equations represent the material property of interest with pre-established units. These equations are directly used as input for the FEA simulation. The equations for the ATR-2E material parameters are:

Perpendicular direction

$$\left(\frac{E}{E_o}\right)_{per} = 10\text{^}(F(-2F^3T - 3.7F^3 + 8.1F^2 - 1.2FT^2 - 7.2F + 0.3T + 3.3))$$

$$DL_{per} = 0.05F^3 + 0.5F^2T + 0.1F^2 + 0.02FT^2 - 0.3FT - 0.1F + 0.02T - 0.001$$

$$CTE_{o_{per}} = 10\text{^}(-0.01T^2 + 0.05T - 5.33)$$

$$\left(\frac{CTE}{CTE_o}\right)_{per} = F(-11.2F^3 - 0.7F^2T + 25.7F^2 + 0.9FT^2 + 2.0FT - 19.4F - 1.8T + 4.5)$$

$$\alpha_{per} = 10\text{^}(-4.6F^3 - 2.4F^2T + 8.9F^2 - 0.5FT^2 + 3.0FT - 5.4F - 0.1T + 1.9)$$

Parallel direction

$$\left(\frac{E}{E_o}\right)_{par} = 10\text{^}(F(-1.1F^3T - 4.1F^3 + 8.9F^2 - 1.2FT^2 - 8.0F + 0.04T + 3.5))$$

$$DL_{par} = 0.02F^3 + 0.4F^2T + 0.1F^2 + 0.01FT^2 - 0.2FT - 0.1F + 0.01T + 0.003$$

$$CTE_{o_{par}} = 10\text{^}(-0.003T^2 + 0.03T - 5.37)$$

$$\left(\frac{CTE}{CTE_o}\right)_{par} = F(-12.4F^3 - 1.8F^2T + 28.3F^2 + 1.0FT^2 + 2.9FT - 20.7F - 1.8T + 4.5)$$

$$\alpha_{par} = 10\text{^}(-4.4F^3 - 1.98F^2T + 8.8F^2 - 0.8FT^2 + 3.1FT - 5.5F - 0.2T + 2.1)$$

where F is the relative dpa ($F = \frac{F_i - F_{min}}{F_{max} - F_{min}}$), F_{min} is 0 (no neutron damage), and T is the relative temperature ($T = \frac{T_i - T_{ambient}}{T_m - T_{ambient}}$). Both F and T are therefore unitless values that range between 0 and 1. The rest of the material parameters have the following units:

Parameter	Unit
Coefficient of thermal expansion (CTE_0) no dpa	$1/℃$
Dimensional change (DL)	$unitless\ \left(\frac{mm}{mm}\right)$
Conductivity (α)	$\frac{W}{m℃}$
Relative Young's Modulus E/E_o	$unitless$
Relative coefficient of Thermal expansion CTE/CTE_o	$unitless$

From the same material source, the reference Young's moduli (no radiation) at room temperature were obtained:

$$E_{o_{par}} = 9167.69\ MPa$$

$$E_{o_{per}} = 8918.94\ MPa$$

Additionally, we obtained from literature the heat transfer coefficients for both the helium in the coolant holes ($h \cong 0.0001 W/mm^2℃$ from [5]) and the TRISO fuel in the fuel holes ($h \cong 0.0004 W/mm^2℃$ from [6]). We took the lowest values available to model a conservative problem; however, the designer can actually describe this material parameter as a function of time and temperature if needed.

2.2.1.3 Boundary Conditions

The following boundary conditions are applied to the graphite core component to represent the operating conditions of a block under high temperatures and exposed to radiation.

- The base (Z=0) is restrained to prevent free body motion.
- The coolant holes start at a temperature of 550°C.
- The fuel holes start at a temperature of 600°C.
- The graphite block starts at room temperature of 20°C.
- The dpa changes with time t and spatial location x, y, z. The function used to describe the dpa assumes that the component has some external radiation source from a neighboring core in the assembly, as was the case in [1]:

$$F_i(x, y, z, t) = 5000\left[\frac{t}{3600}\left(2.5^{-2\frac{x}{1000}}\right)\right]$$

  where time t is in seconds, and the spatial location x is in mm.

All of the above boundary conditions are just approximations of the environment that the graphite core component is subject to, since the main goal of the current work was to establish a proof-of-concept design analysis workflow. Therefore, the description of the boundary conditions can be greatly improved, especially if the actual operating conditions of the graphite core component are known.

2.3 Multiphysics modeling with MOOSE

2.3.1 Overview

The graphite core component was modeled using the open-source finite element software MOOSE for the multi-physics modeling of the component. Unlike most FEA solvers, MOOSE has the ability to easily model complex mathematical models by stacking together the different physics modules needed to represent the problem. As a result, the amount of coding done by the designer is minimal. In this project, the graphite designer only needs to properly establish the boundary conditions in the input file. All the different phenomena: convection, radiation, creep, swelling, etc. are supported by calling different modules, kernels, materials, etc. in the input file.

2.3.2 Specialized source codes for graphite

Since the material properties of graphite are anisotropic and dependent on neutron damage/temperature, additional source pages were generated to handle the unique behavior of graphite. These source files will be publicly available via a git repository in the future.

- AnisoHeatConductionMaterialGraphite → establishes a thermal conductivity in the parallel direction (x) and another thermal conductivity in the perpendicular direction of graphite (y, z).
- GeneralizedKelvinVoigtModelGraphite → Describes the primary and secondary creep behavior of graphite using a Kevin-Voigt material model (the full method is described in [7]). This source file also calculates the anisotropic elastic tensor as a function of dpa.

2.3.3 Input file

The input file as well as the mesh file will be publicly available via a git repository in the future. The overview of the input file is as follows:

- **Set up the tensor mechanics**
    - Small incremental strains
    - Include anisotropic Wigner strains and anisotropic thermal strains
- **Set up functions**
    - Fuel holes temperature
    - Coolant holes temperature
    - dpa in the graphite (described in 2.2.1.3) and its derivative w.r.t. time
    - Parallel conductivity as a function of time and dpa
    - Perpendicular conductivity as a function of time and temperature
- **Set temperature "temp" as a variable with initial value of 20°C**
- **Set auxiliary variables**
- **Set kernel establishing that conductivity is anisotropic**
- **Set auxiliary kernels where all material properties are calculated (as well as the relative dpa and relative temperature needed to calculate them, as described on 2.2.1.2)**
- **Set boundary conditions**
    - Set displacement on z for the base as 0.
    - Prescribe a convective flux to the walls of the coolant holes, using the helium heat transfer coefficient and the coolant hole temperature as input.

- Prescribe a convective heat flux to the walls of the fuel holes, using the TRISO heat transfer coefficient and the fuel hole temperature as input.

- **Set material properties**

  - Set dimensional change DL and relative elastic moduli E/E_o as material properties.

  - Compute the anisotropic thermal strains as: $\varepsilon_{th} = \begin{bmatrix} \left(\frac{CTE}{CTE_o}\right)_{Par} CTE_{o\,Par}(T_i - T_o) \\ \left(\frac{CTE}{CTE_o}\right)_{Par} CTE_{o\,Par}(T_i - T_o) \\ \left(\frac{CTE}{CTE_o}\right)_{Per} CTE_{o\,Per}(T_i - T_o) \\ 0 \\ 0 \\ 0 \end{bmatrix}$

  - Compute the anisotropic Wigner strains as: $\varepsilon_{th} = \begin{bmatrix} DL_{Par} \\ DL_{Par} \\ DL_{Per} \\ 0 \\ 0 \\ 0 \end{bmatrix}$

  - Using the new conductivity module, set anisotropic conductivities as:

$$\alpha[x, y, z] = [\alpha_{Par} \quad \alpha_{Par} \quad \alpha_{Per}]$$

  - Using the new Kevin Voigt module, compute the new compliance tensor:

$$S = \begin{bmatrix} \frac{1}{E_{Par}} & \frac{-v}{E_{Par}} & \frac{-v}{E_{Per}}. & 0 & 0 & 0 \\ \frac{-v}{E_{Par}} & \frac{1}{E_{Par}} & \frac{-v}{E_{Per}}. & 0 & 0 & 0 \\ \frac{-v}{E_{Par}} & \frac{-v}{E_{Par}} & \frac{1}{E_{Per}}. & 0 & 0 & 0 \\ 0 & 0 & 0. & \frac{1}{G} & 0 & 0 \\ 0 & 0 & 0. & 0 & \frac{1}{G} & 0 \\ 0 & 0 & 0. & 0 & 0 & \frac{1}{G} \end{bmatrix}$$

  Where: $G = \left(\frac{E}{E_0}\right)_{Par} E_{0\,Par} + \left(\frac{E}{E_0}\right)_{Per} E_{0\,Per}$, $E_{Par} = \left(\frac{E}{E_0}\right)_{Par} E_{0\,Par}$, and

$$E_{Per} = \left(\frac{E}{E_0}\right)_{Per} E_{0\,Per}.$$

And calculate the primary + secondary creep strains.

- Compute the inelastic stress from creep strains as described in [7], and the elastic stresses from any mechanical load applied on graphite, using the linear elastic model. The thermal and Wigner strains are eigenstrains (residual strains) and therefore do not contribute to the stresses in the material.

- **Create a user object that keeps the Kelvin-Voigt model updated**
- **Set up a simple matrix preconditioning (SMP)**
- **Establish all the executioner options for running the model**
  - Transient model goes up to 120s every 60s. (2 steps total)
  - A Newton solver is used
  - Set up allowable tolerances and PETSC options to help the model converge.
- **Print out an exodus file containing all results**

2.4 ASME Graphite Design Analysis

2.4.1 Overview

The graphite ASME design analysis procedure in the BPVC, Section III, Division 5, allows for three alternative approaches:

a) Simplified assessment - Design of graphite core components that meet the reliability targets based on stress limits.

b) Full assessment - Design of graphite core components that meet the reliability targets based on calculated reliability values derived from the distribution of stresses.

c) Design by test - Design of graphite core components that meet the reliability targets based on experimental proof of the component performance.

The design analysis workflow that we generated concentrates on procedures a) and b) of the BPVC. Both the simplified and full assessment are analyzed jointly during the evaluation of the graphite core component. Figure 6 shows an overview of both assessments, their required input, and the usual reliability targets used in each analysis.

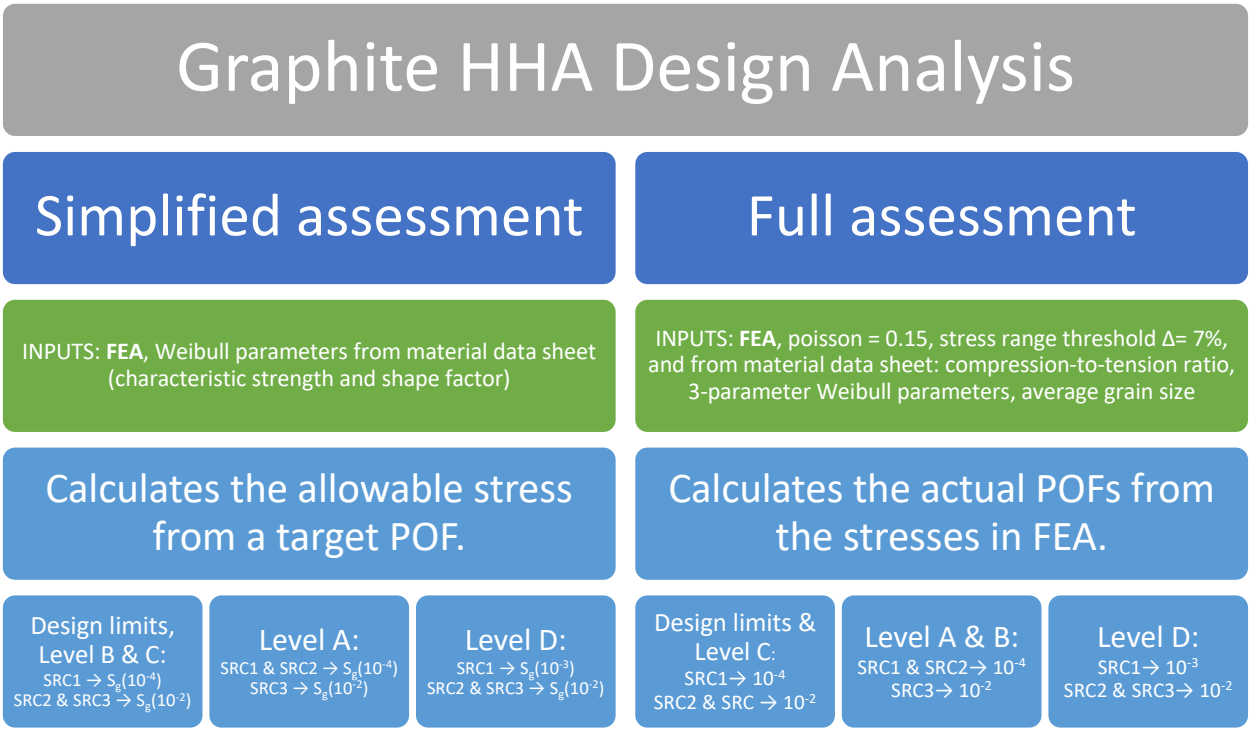

Figure 6: Overview of the HHA graphite design analysis.

2.4.2 Definitions

2.4.2.1 Equivalent stress

The graphite design analysis does not require either the selection of stress classification lines nor the decomposition of loads as in the design rules for metallic components because it directly analyzes the stresses at each point of the FEA model, using an equivalent stress that is based on the Maximum Deformation Energy theory [7], [8]:

$$\sigma_v = \sqrt{\bar{\sigma}_1^2 + \bar{\sigma}_2^2 + \bar{\sigma}_3^2 - 2v(\bar{\sigma}_1\bar{\sigma}_2 + \bar{\sigma}_1\bar{\sigma}_3 + \bar{\sigma}_2\bar{\sigma}_3)} \quad (1)$$

In this equation, v is the Poisson's ratio of graphite (which tends to be approximately 0.15), and:

$\bar{\sigma}_i = f\sigma_i$ for $i = 1,2,3$

σ_1, σ_2, σ_3 are the three principal stresses and the factor f allows the conversion of any compressive stress into an equivalent tensile stress. In other words:

$f = 1$ if σ_i is a tensile stress

$f = R$ if σ_i is a compressive stress

where R is the ratio of mean tensile to mean compressive strength.

2.4.2.2 Weibull distributions

The probability density function (PDF) of a 3-parameter Weibull random variable is:

$$PDF(x) = \frac{\kappa}{\lambda}\left(\frac{x-\theta}{\lambda}\right)^{\kappa-1} \exp\left[-\left(\frac{x-\theta}{\lambda}\right)^{\kappa}\right] \quad (2)$$

Similarly, the cumulative density function (CDF) of a 3-parameter Weibull random variable is:

$$CDF(x) = 1 - \exp\left[-\left(\frac{x-\theta}{\lambda}\right)^{\kappa}\right] \quad (3)$$

In both equations, κ is the shape parameter, λ is the scale parameter, and θ is the location parameter of the Weibull distribution.

The 2-parameter Weibull distributions can be obtained by setting $\theta = 0$:

$$PDF(x) = \frac{\kappa}{\lambda}\left(\frac{x}{\lambda}\right)^{\kappa-1} \exp\left[-\left(\frac{x}{\lambda}\right)^{\kappa}\right] \quad (4)$$

$$CDF(x) = 1 - \exp\left[-\left(\frac{x}{\lambda}\right)^{\kappa}\right] \quad (5)$$

2.4.3 Approaches

2.4.3.1 Simplified assessment

The simplified assessment uses a 2-parameter Weibull distribution to describe the material's reliability curve. The POF can be described as the PDF:

$$POF(S \cong S_g) = \left(\frac{m}{S_c}\right)\left(\frac{S_g}{S_c}\right)^{m-1} \exp\left[-\left(\frac{S_g}{S_c}\right)^{m}\right] \quad (6)$$

where S_c is the characteristic stress (scale), m is the modulus (shape), and S_g is the design equivalent stress. In other words, S_g is an allowable stress that depends on the target POF and the variability in strength of the graphite.

Equation 6 is then used to solve for S_g given a target POF, which is selected based on the Structural Reliability Class (SRC) of the graphite core component and the Design/Service Level of the load (Table 1).

Table 1. POF limits of different SRCs and Design/Service Levels

		Service Limit			
SRC	Design	Level A	Level B	Level C	Level D
SRC-1	10^{-4}	10^{-4}	10^{-4}	10^{-4}	10^{-3}
SRC-2 ([1])	10^{-4} (10^{-2})	10^{-4} (10^{-2})	10^{-4} (10^{-2})	$5\text{x}10^{-2}$	$5\text{x}10^{-2}$
SRC-3	10^{-2}	10^{-2}	10^{-2}	$5\text{x}10^{-2}$	$5\text{x}10^{-2}$

Note [1]: The change in limits is to indicate that the degradation of graphite core components (or increase in stresses) caused by irradiation during service is allowed. The difference between the initial allowable stress value and the allowable stress value in parentheses makes sure that there is margin for material degradation or increase of stresses in service.

The allowable stress $S_g(10^{-n})$ becomes a threshold that determines the pass/fail condition of the graphite core component. If any element in the FEA simulation shows an equivalent stress σ_v (calculated as described in 2.4.2.1) that exceeds the allowable stress S_g, the graphite core component then fails the simplified assessment.

It should be noted that the simplified assessment is always going to be more conservative than the full assessment. Therefore, failing the simplified assessment does not necessarily mean that the design of the graphite core component is not acceptable. A full assessment can be performed to check if the graphite component design is acceptable.

2.4.3.2 Full Assessment

The full assessment uses a 3-parameter Weibull distribution to describe the material's reliability curve. The POF can be described as the CDF:

$$POF(S \leq S_g) = 1 - \exp\left[-\left(\frac{\mathbf{S}-S_o}{S_c-S_o}\right)^m\right] \quad (7)$$

where S_o is the threshold stress (location), S_c is the characteristic strength, $S_c - S_o$ is the adjusted characteristic stress (scale), m is the modulus (shape), and S_g is the target-dependent allowable stress.

The full assessment relies on directly calculating the POF throughout the material and comparing it against a target POF, which requires a more complicated procedure than the simple assessment. Therefore, we rewrite the POF in simpler terms:

$$POF(S \leq S_g) = 1 - \exp[-\mathrm{X}] \quad (8)$$

where:

$$\mathrm{X} = \left(\frac{\mathbf{S}-S_o}{S_c-S_o}\right)^m \quad (9)$$

If the maximum equivalent stress in the component (where the stresses per element σ_v are calculated as described in 2.4.2.1) is less than the 3-parameter Weibull characteristic strength S_c, then the threshold stress S_o is adjusted as:

$$S_o = \frac{\sigma_{\mathrm{v}}^{max}}{S_c} S_o \quad (10)$$

Now, to calculate the POF of the component, the following steps are needed:

1. Rank the integration volumes (elements in FEA) in decreasing order of the equivalent stress σ_{vi}.
2. Truncate the list of elements to those where their equivalent stress is greater than the threshold stress S_o. S_o will need to be adjusted based on Equation 10.
3. Calculate for each element the value of X_i using Equation 9, where $S = \sigma_{vi}$.
4. Group the elements given their volume v_i, starting by the element with the highest equivalent stress. The allocation to groups is based on the following conditions:
    1) The total volume of the group V_I has to exceed a threshold volume V_m:

$$V_I = \sum v_i > V_m \quad (11)$$

where V_m is the cube of the grain size:

$$V_m = (10 Grain_{size})^3$$

The value of the threshold volume V_m tends to be really small for normal graphite (an average grain size of 500 μm gives a value of ~0.5mm^3), so for the mesh generated in 2.2.1.1, the volume groups are comprised of about 2 to 3 elements.

2) The range of values X within the group (for example, group I), has to exceed 7% (which is the stress range parameter Δ in the ASME code):

$$\frac{\max(X_I) - \min(X_I)}{\min(X_I)} > 7\% \tag{12}$$

5. For each group of elements, we calculate:

$$A_I = \sum \frac{X_i v_i}{V_I} \tag{13}$$

where X_i and v_i are the values of each element, and V_I is the volume of the group.

6. And we use A to calculate the probability of survival (POS) L per group:

$$L_I = e^{-A_I} \tag{14}$$

7. We can then calculate the POS of the graphite core component by multiplying the POS of all groups:

$$L = \prod_I L_I \tag{15}$$

8. The POF of the component can then be calculated accordingly:

$$POF = 1 - L \tag{16}$$

This value is compared against the allowed POF limit selected in Table 1, and a pass/fail of the graphite core component is issued.

3 Results

3.1 Description of analysis software

The output *.exo file that results from the FEA simulation is directly used as input for the design analysis software. This software is comprised of a python library with all the calculations described in sections 2.4.2 - 2.4.3, and a python running script that calls the calculation methods when needed. The software will be publicly available via a git repository in the future.

3.1.1 Inputs

The software only needs as input the following variables:

1. The name of the *.exo input file (can include full location path)
2. The compression-to-tension ratio R (from material data sheet)
3. The 2-parameter Weibull parameters (from material data sheet)
4. The 3-parameter Weibull parameters (from material data sheet)
5. The average graphite grain size (in mm, from material data sheet)

These variables can be explicitly written down in the running script "RUN_assessment.py" in the input data block:

```
################################################################################
#                    ASME BPVC-III-5 Analysis for graphite
#                  Subsection HH subpart A (HHA-3000 DESIGN)
################################################################################
import numpy as np
import shutil
import netCDF4
from HHAanalysis import simple, full, hhamath, writer
################################ INPUT DATA ####################################
infile  = 'ETU10_moose_slice_out2.e'
compratio = 0.264 #Compression to tension conversion ratio

###### parameters needed for Simple Analysis ######
# 2-parameter Weibull parameters (from Data Sheet)#
Sc = 21.56  # characteristic strength Sc(scale) [MPa]
m  = 5.78   # shape factor m

####### parameters needed for Full Analysis #######
# 3-parameter Weibull parameters (from Data Sheet)#
S0 = 8.25   # Threshold value So(location)      [MPa]
Sc = 21.56  # characteristic strength Sc(scale) [MPa]
m  = 5.78   # shape factor m
# Other values (from Data Sheet) #
GG_size = 0.04     # Average graphite grain size [mm]

################################################################################
```

Figure 7: View of the input data section inside the running python script

3.1.2 Outputs

This analysis software outputs two results:

1. An output *.exo file where any failing locations are highlighted given the simplified/full assessment, as seen in Figure 8.
2. A summary of both simple and full assessments using all POF limits listed in Table 1, as seen in Figure 9.

Each element in the graphite core component is flagged as PASS (0) or FAIL (1) based on the following:

- Simplified Assessment: The local equivalent stress surpasses the allowable stress S_g.
- Full Assessment: The local POF (calculated from the local POS) surpasses the limit POF.

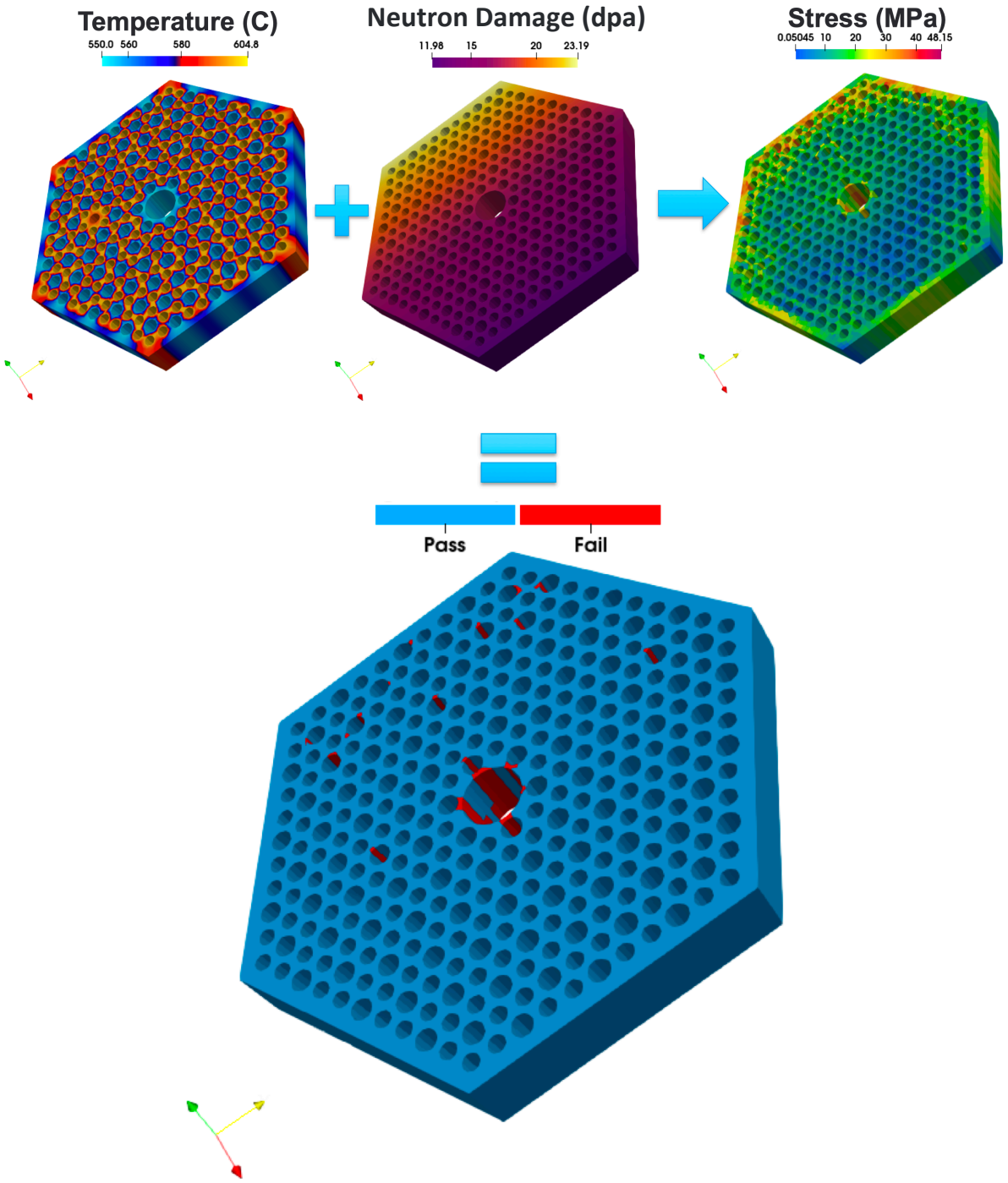

Figure 8: View of the failing locations in the geometry, for a simplified assessment with an $S_g(5x10^{-2})$. The pass/fail plots for all limits and assessments are readily available in the output file.

The results summary lists all evaluations at each time step of the simulation, as shown in Figure 9. That way, the designer can model the actual load history of the graphite core component over time and see the conditions in which the design is compliant (or not) with the ASME BPVC graphite design rules.

```
[anicolas@c355125 GraphiteFEA]$ python3 RUN_assessment.py
Time is =  0.0
Max Equivalent Stress [MPa] =  0.0
from Simple Assessment @ 5e-2 Max Allowable stress is = [25.09] MPa, it PASSES
from Simple Assessment @ 1e-2 Max Allowable stress is = [10.88] MPa, it PASSES
from Simple Assessment @ 1e-3 Max Allowable stress is = [6.69] MPa, it PASSES
from Simple Assessment @ 1e-4 Max Allowable stress is = [4.13] MPa, it PASSES

Probability of Failure [PoF] =  0.0 %
from Full Assessment with Max Probability of Failure of @ 5e-2, it PASSES
from Full Assessment with Max Probability of Failure of @ 1e-2, it PASSES
from Full Assessment with Max Probability of Failure of @ 1e-3, it PASSES
from Full Assessment with Max Probability of Failure of @ 1e-4, it PASSES

Time is =  60.0
Max Equivalent Stress [MPa] =  967.89
from Simple Assessment @ 5e-2 Max Allowable stress is = [25.09] MPa, it PASSES
from Simple Assessment @ 1e-2 Max Allowable stress is = [10.88] MPa, it PASSES
from Simple Assessment @ 1e-3 Max Allowable stress is = [6.69] MPa, it FAILS
from Simple Assessment @ 1e-4 Max Allowable stress is = [4.13] MPa, it FAILS

Probability of Failure [PoF] =  0.4219 %
from Full Assessment with Max Probability of Failure of @ 5e-2, it PASSES
from Full Assessment with Max Probability of Failure of @ 1e-2, it PASSES
from Full Assessment with Max Probability of Failure of @ 1e-3, it FAILS
from Full Assessment with Max Probability of Failure of @ 1e-4, it FAILS

Time is =  120.0
Max Equivalent Stress [MPa] =  1935.78
from Simple Assessment @ 5e-2 Max Allowable stress is = [25.09] MPa, it PASSES
from Simple Assessment @ 1e-2 Max Allowable stress is = [10.88] MPa, it FAILS
from Simple Assessment @ 1e-3 Max Allowable stress is = [6.69] MPa, it FAILS
from Simple Assessment @ 1e-4 Max Allowable stress is = [4.13] MPa, it FAILS

Probability of Failure [PoF] =  58.951 %
from Full Assessment with Max Probability of Failure of @ 5e-2, it FAILS
from Full Assessment with Max Probability of Failure of @ 1e-2, it FAILS
from Full Assessment with Max Probability of Failure of @ 1e-3, it FAILS
from Full Assessment with Max Probability of Failure of @ 1e-4, it FAILS
```

Figure 9: Summary overview of all design assessments

4 Conclusions and Future Work

This report has presented a complete design analysis workflow that allows the designer to assess a graphite core component against the Section III, Division 5, HHA-3000 design criteria. This framework can be used by designers with a basic experience in FEA and python, and all the tools necessary to use this framework will soon be available in git repositories. By using the open-source software MOOSE, we converted the complex process of modeling the physics and material behavior of graphite into a simple system that only requires the input of material properties in the form of polynomial functions. In conclusion, the modeling and analysis of graphite core components have now been streamlined and largely automated, and some avenues for future work have been opened from the results of this work.

An avenue for future work would be validating the results from FEA simulations with experimental characterizations. This work would require a complex set of experiments, in which the graphite component would need to be actually subjected to irradiation and high temperatures at the time of its characterization. Given the level of complexity that such an experiment entails, this future work would require highly knowledgeable experimentalists and the access to facilities that can handle highly aggressive environments. The difficulty of obtaining access to these requirements also explains why most of the methodologies developed to model graphite tend to be validated by demonstrating that the material behavior has been adequately characterized from experimental data from simple stress state, which is what we did during the early stages of this work.

Another avenue that may be of interest is obtaining the operational history of graphite components and assemblies, and examining the actual locations of fracture at the end of the component's service life. The experimental characterization of failure initiation could then be compared against the simulated counterpart, which we then could use to evaluate the workflow's ability to predict both the onset and the location of failure.

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REFERENCES

[1] Robert Bratton, "Modeling Mechanical Behavior of a Prismatic Replaceable Reflector Block (INL/EXT-09-15868 Revision 0)," Idaho National Laboratory, Apr. 2009. doi: 10.2172/961925.

[2] J. W. Sterbentz, P. D. Bayless, L. O. Nelson, H. D. Gougar, J. Kinsey, and G. Strydom, "High Temperature Gas-Cooled Test Reactor Point Design: Summary Report (INL/EXT-16-37661 Revision 1)," Idaho National Laboratory, Mar. 2016. doi: 10.2172/1260453.

[3] USNC, "Nuclear Graphite Interactive Material Model and Simulation Environment Model," 2018. https://github.com/ultra-safe-nuclear-corporation/NGIMASEM.git.

[4] G. Haag, "Properties of ATR-2E Graphite and Property Changes due to Fast Neutron Irradiation (Jülich-4183)," Institut für Sicherheitsforschung und Reaktortechnik, 2005. doi: 0944-2952.

[5] Q. Liu, Z. Zhao, and K. Fukuda, "Transient heat transfer for forced flow of helium gas along a horizontal plate with different widths," *Int. J. Heat Mass Transf.*, vol. 75, pp. 443–441, 2014.

[6] R. Stainsby, "Investigation of Local Heat Transfer Phenomena in a Pebble bed HGTR Core (NR001/RP/002 R01)," AMEC NSS Limited, 2009.

[7] C. Erasmus, S. Kok, and M. P. Hindley, "Significance of primary irradiation creep in graphite," *J. Nucl. Mater.*, vol. 436, no. 1–3, pp. 167–174, 2013.

[8] M. P. Hindley *et al.*, "A numerical stress based approach for predicting failure in NBG-18 nuclear graphite components with verification problems," *J. Nucl. Mater.*, vol. 436, no. 1–3, pp. 175–184, 2013.

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